

# MSDE

## Molecular Systems Design & Engineering rsc.li/molecular-engineering

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Chris Erik Mohn *et al.*,  
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10, 519.



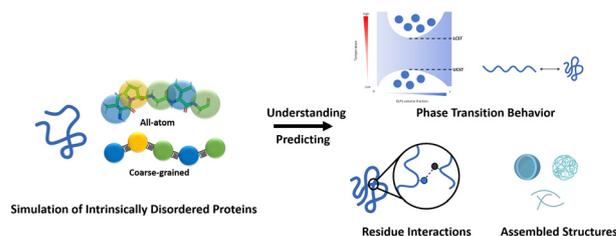
**Inside cover**  
See Bret D. Ulery *et al.*,  
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### REVIEW

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#### Toward understanding biomolecular materials comprising intrinsically disordered proteins *via* simulation and experiment

Bin Wang, Tianren Zhang, Sirui Shen, Darrin J. Pochan,  
Jeffery G. Saven\* and Kristi L. Kiick\*

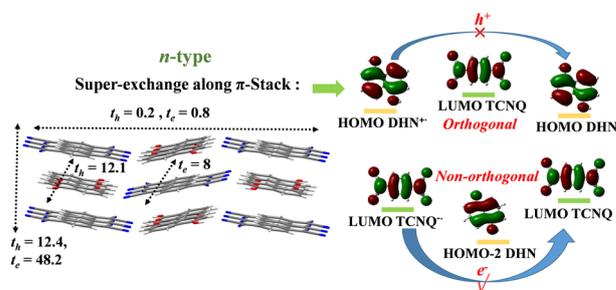


### PAPERS

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#### Elucidating the role of charge transfer on semiconductor properties in a new donor-acceptor cocrystal 1,5-dihydroxynaphthalene : TCNQ

Arkalekha Mandal,\* Chris Erik Mohn,\*  
Carl Henrik Görbitz, Melania Rogowska and Ola Nilsen





# RSC Applied Polymers

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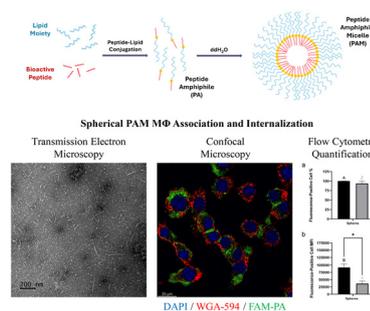
Fundamental questions  
Elemental answers



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## Vasoactive intestinal peptide amphiphile micelle material properties influence their cell association and internalization

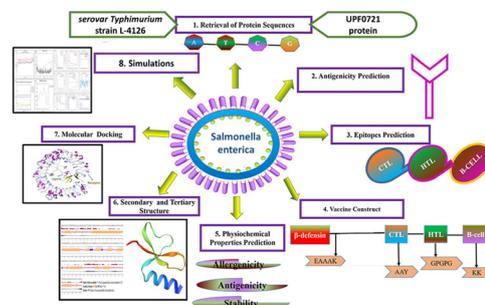
Xiaofei Wang, Agustin T. Barcellona, Fateme Nowruzi, Kambrie M. Brandt, Megan C. Schulte, Luke E. Kruse, Eric Dong, Adam G. Schrum, Esma S. Yolcu and Bret D. Ulery\*



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## Designing a multi-epitope vaccine targeting UPF0721 of meningitis-causing *Salmonella enterica* serovar Typhimurium strain L-4126 by utilizing immuno-informatics and *in silico* approaches

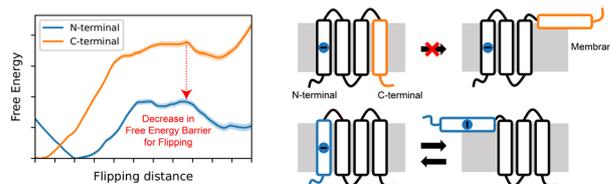
Elham Mohammed Khatrawi, Syed Luqman Ali,\* Syed Yasir Ali, Aigul Abduldayeva\* and Alaa S. Alhegaili



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## Bioinspired design rules for flipping across the lipid bilayer from systematic simulations of membrane protein segments

ByungUk Park and Reid C. Van Lehn\*



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## DynaMate: leveraging AI-agents for customized research workflows

Orlando A. Mendible-Barreto, Misael Díaz-Maldonado, Fernando J. Carmona Esteva, J. Emmanuel Torres, Ubaldo M. Córdova-Figueroa and Yamil J. Colón\*

```

1 class HelloWorld_inps(BaseModel):
2     message: str = Field(description="Message to print")
3     times: int = Field(description="Amount of times to print message")
4
5
6 def hello_world(message: str, times: int):
7     return message * times
8
9
10 HelloWorld_Tool = StructuredTool.from_function(
11     func=hello_world,
12     name="HelloWorld",
13     description="Prints a message a number of times",
14     args_schema=HelloWorld_inps,
15     return_direction=False,
16     handle_error=True,)

```

